Transport, Growth, Decay and Sorption of Microorganisms and Nutrients through Porous Media: A Simulation with COMSOL

D.A. Lopez-Falcon[*,1], M.A. Diaz-Viera[1], and A. Ortiz-Tapia[1]
[1]Instituto Mexicano del Petroleo (IMP): Programa de Recuperacion de Hidrocarburos
*Corresponding author: Eje central Lazaro Cardenas 152, A.P. 14-805, Mexico 07730 D.F., dalopez@imp.mx

Abstract: Fate of microorganisms in porous media has very important applications in many branches of environmental and petroleum science and engineering, among others; however, concurrently it is a very complex and interacting phenomenon mainly because microorganisms are living. Applying the systematic modeling approach to continuum systems, we derive a model that include net flux of microorganisms and nutrients by convection and dispersion, growth and decay rates of microorganisms, chemotactic movement and nutrient consumption, adsorption of microorganisms and nutrients on rock grain surfaces, as well as desorption of microorganisms. Porosity reduction due to cell adsorption is considered. We use the Solute Transport application of the Earth Science Module in COMSOL Multiphysics to implement a numerical solution of the model. The numerical simulations reproduce results previously reported elsewhere; moreover, we show the spatial-temporal distribution of microorganisms and nutrients along the system and time. We point out the complementary role of the spatial-temporal distribution of components with breakthrough curves to analyze the behavior of both fluent and adsorbed components.

Keywords: Microorganism, Sorption, Transport model, Porous media, Breakthrough curve.

1. Introduction

Transport of microorganisms through porous media governs many phenomena in bioremediation of environmental pollution problems and microbial enhanced oil recovery. The aim of this work is to investigate the effects of some transport parameters on breakthrough curves as well as on spatial distribution of components transported through a porous medium by a fluid phase.

1.1 Description of the Problem

We are considering the transport of microorganisms and nutrients by water injected through a porous medium in a laboratory scale.

The first system analyzed is from Tan et al. [1]. A 0.3 m long column packed with aquifer sand. A peristaltic pump was used to supply liquids at constant upward flow velocities. A pulse type boundary condition was chosen for all cases. The sand column was saturated with percolating sterile deionized water prior to the breakthrough curve (BTC) was obtained. To measure the BTC of microorganisms, deionized water was replaced for 1 hour by the microorganism suspension, and then the flow of sterile deionized water was resumed. We will show the simulated sodium chloride BTCs for three flow velocities; in agree with Sen et al. [2], we obtain dispersion coefficients two orders of magnitude greater than which obtained by Tan et al.. Following Sen et al., we only show the BTC of microorganisms used by them to validate their model. We can observe some differences among microorganism's BTCs as we implement models with varying features.

The second system discussed is from Chang et al. [3]. A sample of rock (usually called core). In this case, we simulate a continuous and simultaneous injection both of microorganisms and nutrients until a steady state is obtained. We observe that for a large enough time, a practically full consumption of nutrients by microorganisms is established. The planktonic and the sessile microorganisms have a maximum concentration at approximately three tenths and one sixth of the system length from the injection side, respectively.

2. Systematic Modeling Approach

The local balance equations obtained from the systematic modeling approach to continuum systems are [4]:

$$\boxed{\frac{\partial \psi_\gamma^\alpha}{\partial t} + \vec{\nabla}\cdot(\psi_\gamma^\alpha \vec{v}^\alpha - \vec{\tau}_\gamma^\alpha) = g_\gamma^\alpha; \quad \forall \vec{x} \in B(t)} \qquad (1)$$

where ψ_γ^α is the intensive property associated with γ component in phase α of our interest; $\vec{v}^\alpha$ is the mean velocity of that phase, $\vec{\tau}_\gamma^\alpha$ is the flux of the property through the boundaries of the system, and g_γ^α represents the sources on the region occupied by the body, $B(t)$.

Even though, these are the basic governing equations for a wide diversity of continuum systems, they are not enough to completely define a model. To get *complete models*, in addition to the basic equations, one first requires sufficient *constitutive laws* linking intensive properties between themselves and defining the sources, g_γ^α, the fluxes $\vec{\tau}_\gamma^\alpha$ and phase velocities $\vec{v}^\alpha$ in terms of them. Moreover, proper initial and boundary conditions should be specified (and they must be satisfied) for the intensive properties, such that a well posed problem is defined. This means that the solution of the problem exists and is unique.

3. Derivation of the Model

In general, we employ the following constitutive laws: Darcy's velocity $\vec{u}^\alpha = \phi^\alpha \vec{v}^\alpha$ which characterizes the advection, where ϕ^α is the volume fraction occupied by the α phase. Fick's law, which can be written in a generalized sense as $\vec{\tau}_\gamma^\alpha = \mathbf{D}_\gamma^\alpha \cdot \nabla \psi_\gamma^\alpha$, where $\mathbf{D}_\gamma^\alpha$ is a tensor which includes several conduction processes such as diffusion and dispersion. The sources g_γ^α consist of various types of physicochemical and biological reactions, injection/production rates and other sources.

In particular, to construct the model we assume that:

- The system has three phases: fluid water, with $\vec{v}^w = \vec{v}$; static biofilm and solid, with $\vec{v}^{b,r} = 0$.
- The system has four components: water is only in water phase, rock is only in solid phase, microorganisms are partitioned among water and biofilm phases, and so are the nutrients between water and solid phases.
- The porous medium is saturated, so $\phi^w = S^w \phi = \phi$ where the water saturation is $S^w = 1$ and the porosity is ϕ; as well as the medium is isotropic, so $\mathbf{D}_\gamma^\alpha = D_\gamma^\alpha \mathbf{I}$ is a diagonal matrix.
- The conduction of components is due to hydrodynamic dispersion, so $D_\gamma^w = \left(\alpha |\vec{v}| + \tau D_{m_\gamma}\right)$ where the dispersivity is α, the tortuosity is $\tau < 1$ and the molecular diffusion is D_{m_γ}.
- Microorganisms and nutrients have biological interaction, as growth Monod equation [5]: $\mu = \dfrac{\mu_{\max} c_n^w}{K_{m/n} + c_n^w}$, where the maximum specific growth rate is $\mu_{\max}$, Monod constant for the nutrient is $K_{m/n}$, and the water nutrient's concentration is c_n^w; and linear chemotactic velocity, as [6]: $\vec{v}^c = k_c \nabla\left(\ln c_n^w\right) = k_c \nabla c_n^w / c_n^w$, where the chemotactic sensitivity coefficient is $k_c = f s^2 R_t / 4$, while the differential tumbling frequency is f, the 1D swimming speed is s, and the number of receptors is R_t.
- Microorganisms have linear decay: $k_d \rho_m \sigma$ for sessile ones and $k_d \phi c_{pm}^w$ for planktonic. Here, the cell's specific decay rate is k_d and we assume that it is the same for both, microorganism's density is ρ_m, the volume of sessile microorganisms by unit volume of bulk soil is σ, and the water planktonic microorganism's concentration is c_{pm}^w.
- Nutrients and solid have physicochemical interaction, as a preferred type of adsorption isotherm: Linear, $c_n^s = K c_n^w$; Freundlich [7], $c_n^s = K_F c_n^{w^N}$; or Langmuir [8,9], $c_n^s = \dfrac{K_L \bar{s} c_n^w}{1 + K_L c_n^w}$.
- Microorganisms and solid have physicochemical interaction, as a irreversible limited desorption: $k_r \rho_m \left(\sigma - \sigma_{irr}\right)$ for $\sigma > \sigma_{irr}$ and 0 for

$\sigma < \sigma_{irr}$, where the desorption rate coefficient is k_r, and the minimum sessile cell concentration is σ_{irr}, which accounts for cells that are irreversibly adsorbed within the porous medium.

- Microorganisms have quasi-linear adsorption on solid: $k_a(\phi_0 - \sigma)c^w_{pm}$, where the adsorption rate coefficient is k_a.
- Porosity reduction due to cell adsorption is considered as: $\phi = (\phi_0 - \sigma)$, where the initial porosity is ϕ_0.
- Microorganisms are uniformly suspended in water: $\rho_m \simeq \rho_w$, such that sedimentation is negligible: $\vec{v}^g = 0$.
- Flow is assumed to be at steady state; hence a constant flow velocity is imposed.

We summarize part of the above assumptions in table 1.

Table 1: Intensive properties associated with mass of components

Phase (α)	Component (γ)	Intensive Property
Water ($\alpha = w$)	Water ($\gamma = w$) Planktonic ($\gamma = pm$) Nutrients ($\gamma = n$)	$\phi\rho_w$ ϕc^w_{pm} ϕc^w_n
Biofilm ($\alpha = b$)	Sessile ($\gamma = sm$)	$c^b_{sm} = \rho_m\sigma$
Solid ($\alpha = s$)	Rock ($\gamma = r$) Nutrients ($\gamma = n$)	$\rho_{r_b} = (1-\phi)\rho_{r_p}$ $\rho_{r_b} c^s_n$

Where the water density is ρ_w and the bulk soil density is ρ_{r_b} when the particle density is ρ_{r_p}.

4. Governing Equations

Applying the systematic modeling approach to continuum systems (summarized by equation (1)) and considering the previous assumptions, we obtain the following governing equations for the problems described in subsection 1.1:

Microorganisms

Planktonic (in water)

$$\frac{\partial}{\partial t}\left(\phi c^w_{pm}\right) + \nabla\cdot\left(\phi c^w_{pm}\vec{v}^t - \mathbf{D}^w_{pm}\cdot\nabla\left(\phi c^w_{pm}\right)\right) = \\ = \left(\mu - k_d - k_a\right)\phi c^w_{pm} + k_r\rho_m\left(\sigma - \sigma_{irr}\right) \quad (2)$$

where $\vec{v}^t = \vec{v}^w + \vec{v}^c + \vec{v}^g$ is the total velocity composed by adding the mean water, chemotactic, and sedimentation velocities, respectively.

Sessile (in biofilm)

$$\frac{\partial}{\partial t}\left(\rho_m\sigma\right) = \\ = \left(\mu - k_d - k_r\right)\rho_m\sigma + k_a\phi c^w_{pm} + k_r\rho_m\sigma_{irr} \quad (3)$$

Remember that desorption term exist only if $\sigma > \sigma_{irr}$.

Nutrients

Total (in water and rock)

$$\left(\phi + \rho_{r_b}\partial_{c^w_n}c^s_n\right)\frac{\partial}{\partial t}c^w_n + \\ +\nabla\cdot\left(\vec{u}^w c^w_n - \mathbf{D}^w_n\cdot\nabla\left(\phi c^w_n\right)\right) = \\ = -\mu\left(\phi c^w_{pm} + \rho_m\sigma\right)/Y_{m/n} \quad (4)$$

Select one of the predefined adsorption isotherm.

Additionally to this system, we need a set of initial and boundaries conditions. We use the following ones:

Initial condition:

$$c^w_{pm}\big|_{t=0} = \sigma\big|_{t=0} = c^w_n\big|_{t=0} = 0 \quad (5)$$

Inlet boundary condition (general Neumann):

$$-\hat{n}\cdot\left[\phi c^w_\gamma\vec{v} - \mathbf{D}^w_\gamma\cdot\nabla\left(\phi c^w_\gamma\right)\right]\Big|_{x=0} = \hat{n}\cdot\phi c^w_{\gamma_0}\vec{v} \quad (6)$$

where $\gamma = pm, n$ and $c^w_{\gamma_0} \neq 0$ only during the injection of the pulse, i.e., for $0 < t < t_{inj}$.

Outlet boundary condition (advective flux):

$$-\hat{n}\cdot\left[-\mathbf{D}_{\gamma}^{w}\cdot\nabla\left(\phi c_{\gamma}^{w}\right)\right]_{x=x_L}=0 \qquad (7)$$

5. Numerical Model

The previously derived model is a mathematically defined system of three fully coupled partial differential equations (2)-(4), the last of which can be nonlinear; for three variables: c_{pm}^{w}, σ and c_{n}^{w}. We implement the corresponding numerical model using the powerful computational environment provided by COMSOL Multiphysics [11].

5.1 Implementing the Model of BTCs for Sandy Column Simulations

First of all, we perform numerical simulations in 1D of the BTCs of sodium chloride (tracer, $\gamma = t$) for three flow velocities to determine the dispersion coefficient, D_t^w. The domain is a 0.3 m line segment. The mesh consists of 960 elements. We use the default setting, i.e. quadratic Lagrange polynomials to interpolate and the UMFPack as linear system solver; in consequence there are 1921 degrees of freedom.

In this case there is only one equation to solve:

$$\frac{\partial}{\partial t}\left(\phi c_t^w\right)+\frac{\partial}{\partial x}\left(\phi c_t^w v-D_t^w\frac{\partial}{\partial x}\left(\phi c_t^w\right)\right)=0 \qquad (8)$$

with the following initial and boundaries conditions:

$$\begin{aligned} &c_t^w\big|_{t=0}=0\\ &\phi c_t^w v-D_t^w\frac{\partial}{\partial x}\left(\phi c_t^w\right)\Big|_{x=0}=-\phi c_{t_0}^w v \qquad (9)\\ &-D_t^w\frac{\partial}{\partial x}\left(\phi c_t^w\right)\Big|_{x=x_L}=0 \end{aligned}$$

where $c_{t_0}^w\neq 0$ only during the pulse injection, i.e., for $0<t<t_{inj}$.

We used data from Tan et al., shown in table 2.

Secondly, assuming that the dispersion coefficient for planktonic microorganisms is the same as the dispersion coefficient for tracer previously obtained: $D_{pm}^w=D_t^w$, we proceed to establish the adsorption and desorption rate coefficients, k_a and k_r, performing a numerical simulation of the BTC of microorganisms suspended in deionized water for a flow velocity of $\vec{v}=0.2$ mm/s and injected cell concentration of $c_{pm_0}^w=1.2\times10^8$ cells/mL. The domain and its partition remains the same as above but degrees of freedom are doubled, because in this case there are two equations to solve, (2) and (3) with μ and k_d set to zero, as growth and decay are neglected; and $\vec{v}^t=\vec{v}$ as chemotactic and sedimentation velocities are null, thus obtaining

$$\begin{aligned} &\frac{\partial}{\partial t}\left(\phi c_{pm}^w\right)+\nabla\cdot\left(\phi c_{pm}^w\vec{v}-\mathbf{D}_{pm}^w\cdot\nabla\left(\phi c_{pm}^w\right)\right)=\\ &=k_r\rho_m\left(\sigma-\sigma_{irr}\right)-k_a\phi c_{pm}^w \qquad (10)\\ &\frac{\partial}{\partial t}\left(\rho_m\sigma\right)=k_a\phi c_{pm}^w+k_r\rho_m\left(\sigma-\sigma_{irr}\right) \qquad (11) \end{aligned}$$

with the same initial and boundary conditions as above, but $\gamma=pm$ instead of $\gamma=t$ and adding one initial condition:

$$\sigma\big|_{t=0}=0 \qquad (12)$$

and using a minimum sessile cell concentration of $\sigma_{irr}=0.02$. Remember that the desorption term exist only if $\sigma>\sigma_{irr}$.

Table 2: Input data for tracer BTCs in sandy column [1]

Parameter	Value
Porosity	$\phi=0.38$
Water velocities	$v=0.05,0.1,0.2$ mm/s
Injected concentration	$c_{t_0}^w=0.01$ mol/L
Injection time	$t_{inj}=1$ h
Column length	$x_L=0.3$ m

5.2 Implementing the Model of MEOR Core Flooding Simulation

Now we simulate a 1D core flooding with microorganisms and nutrients simultaneously and continuously. The domain is now a 0.25 m line segment. The mesh consists of 120 elements. We use the default setting again, such that now there are 723 degrees of freedom.

In this problem we use the complete model, equations (2)-(4), with $\vec{v}^t=\vec{v}$ as chemotactic and sedimentation velocities are null, and $c_n^s=0$

as there are not nutrients adsorption. We used data from Chang et al., shown in table 3.

Table 3: Input data for BTCs and distributions of nutrients and microorganisms in core flooding [3]

Parameter	Value
Porosity	$\phi = 0.2295$
Injection rate	$u = 1$ ft/day
Nutrients dispersion coefficient	$D_n^w = 0.0083$ ft^2/day
Microorganisms dispersion coefficient	$D_{pm}^w = 0.0055$ ft^2/day
Maximum specific growth rate	$\mu_{\max} = 8.4$ day^{-1}
Monod constant	$K_{m/n} = 0.5$ lb/ft^3
Yield coefficient	$Y_{m/n} = 0.5$
Specific decay rate	$k_d = 0.22$ day^{-1}
Desorption rate	$k_r = 37$ day^{-1}
Adsorption rate	$k_a = 25$ day^{-1}
Minimum sessile cell	$\sigma_{irr} = 0.003$
Nutrients injected concentration	$c_{n_0}^w = 2.5$ lb/ft^3
Microorganisms injected concentration	$c_{pm_0}^w = 1.875$ lb/ft^3
Injection time	$t_{inj} = 24$ h
Column length	$x_L = 0.25$ m

6. Discussion of Experimental Results

Next, we show and discuss simulation results for the two systems analyzed in this work.

6.1 BTCs for Sandy Column Simulations

Simulated sodium chloride BTCs for three flow velocities are shown in Fig. 1. We agreed with Sen et al., as we obtain dispersion coefficients $D_t^w \sim 10^{-4}$ m^2/s, i.e. two orders of magnitude greater than those obtained by Tan et al.. Following Sen et al., we show in Fig. 2 the BTC of microorganisms used by them to validate their model. We can observe some difference among microorganisms BTCs as we implement models with varying features. The model (black curve in Fig. 2) corresponding to adding all differences observed respect to Sen et al. (blue curve), namely, a different inlet boundary condition, include porosity reduction due to cell adsorption, as well as we infer that the conditional desorption was omitted by them in their implementation of transport equation for sessile microorganisms (note the flatness in the blue curve versus the inflection points at $c_{pm}^w / c_{pm_0}^w \approx 0.2$ in the red and the black curves of Fig. 2).

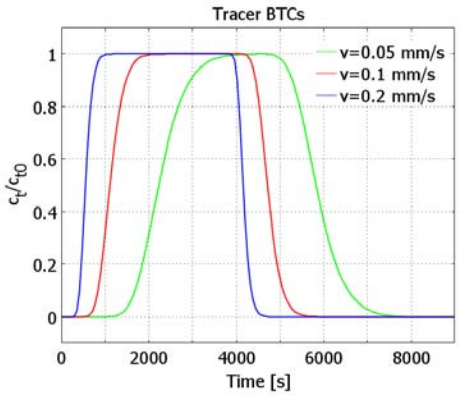

Figure 1. BTCs of sodium chloride.

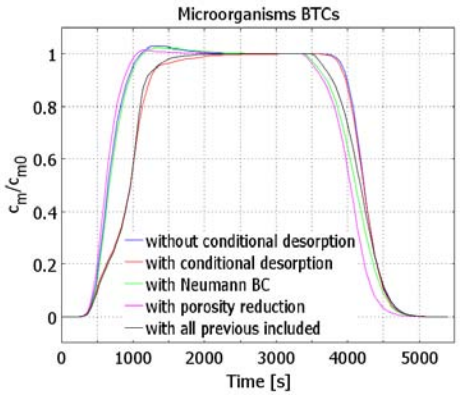

Figure 2. BTCs of microorganisms.

Additionally, we show in Figs. 3 and 4, the spatial-temporal distribution of adsorbed microorganisms (along the column and every minute) with and without conditional desorption. In the first case, we observe that there is an interesting behavior, mainly around $x = 0.18$ m for $13 < t < 25$ minutes. We think that this behavior (such as "clogging") is due to the interaction between adsorbed and flowing microorganisms quantified by means of conditional desorption. Meanwhile, the lack of implementation of the conditional desorption

leads to unphysical adsorption ($\sigma \neq 0$ at $t = 1$ minute and $x = x_L$, bottom curve of Fig. 4).

It is evident the relevance of obtaining the spatial distribution of components (mainly, the adsorbed ones) besides the BTCs, because the latter will not give us direct information about the former.

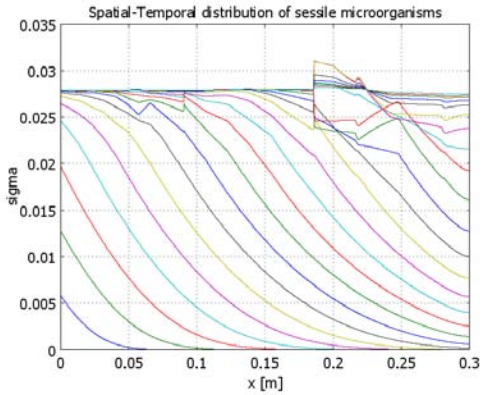

Figure 3. Spatial-Temporal distribution (every minute up to the 25th) of adsorbed microorganisms with conditional desorption.

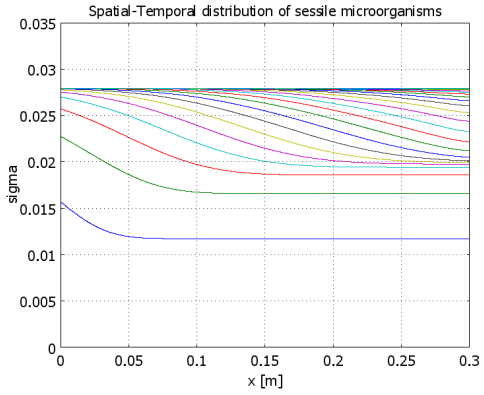

Figure 4. As Fig. 3, without conditional desorption.

6.2 MEOR Core Flooding Simulation

Simulated nutrients and microorganisms BTCs for a continuous and simultaneous 1D core flooding are shown in Fig. 5. We observe a clear difference between the nutrients BTCs as practically no BTC exists in the case when it is not considered conditional desorption, Neumann BC, and porosity reduction; meanwhile, between microorganisms BTCs we note a little plateau (a kind of "quasi-stationary state") of almost 45 minutes at around 5 hours of injection, which we explain as a dynamical equilibrium in growth and sorption of the microorganisms along the core.

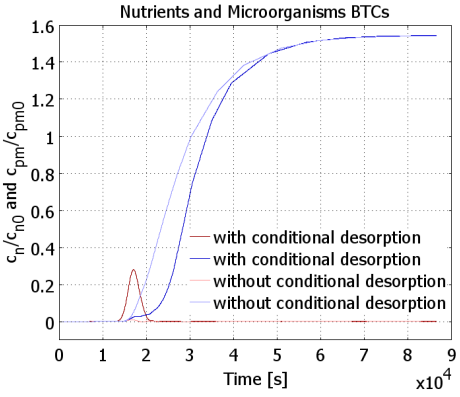

Figure 5. BTCs of nutrients (red curves) and microorganisms (blue curves).

Moreover, we show in Fig. 6 the nutrient and planktonic microorganism distributions along the core for some selected times.

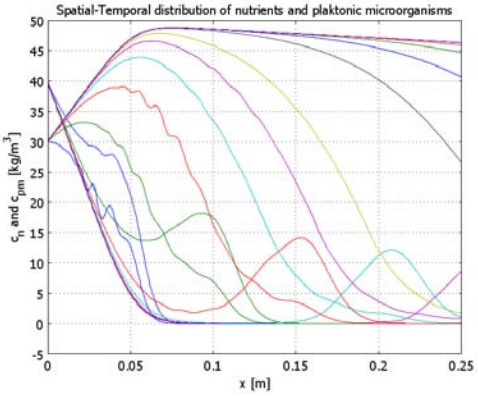

Figure 6. Spatial-Temporal distribution (every hour up to the 6th, and every 3 hours hereafter) of nutrients and planktonic microorganisms (rising from 30kg/m^3).

Finally, we present in Fig. 7 the distribution of sessile microorganisms along the core for the same times above.

In Figs. 6 and 7, we observe steady states: for a time of about 6 hours a practically full consumption of nutrients is established, whereas for a time of about 24 hours an asymptotic value of microorganism concentration is reached. Additionally, we observe that planktonic and

sessile microorganisms have maximum concentration values of $c_{pm}^{w} = 48.85$ kg/m^3 and $\sigma = 1.09\%$ at 0.074 m and 0.041 m (approximately three tenths and one sixth of the system length from the injection side), respectively.

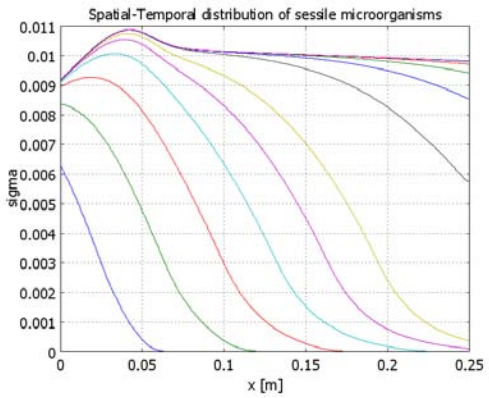

Figure 7. Spatial-Temporal distribution (as above) of sessile microorganisms.

7. Conclusions

Applying the systematic modeling approach to continuum systems, we derive a model that include the net flux of microorganisms and nutrients by convection and dispersion, growth and decay rates of microorganisms, chemotactic movement and nutrient consumption, adsorption of microorganisms and nutrients on rock grain surfaces, as well as desorption of microorganisms. Porosity reduction due to cell adsorption is considered.

For sandy column, we conclude that it is evident the relevance of obtaining the spatial distribution of components (mainly, adsorbed ones) besides the BTCs, because the latter will not give us direct information about the former. Phenomena such as "clogging" could be observed if the interaction between adsorbed and flowing microorganisms quantified by means of conditional desorption is included, else, unphysical adsorption is obtained.

For core flooding, we observe that a practically full consumption of nutrients is established earlier than an asymptotic concentration of microorganisms. The planktonic and the sessile microorganisms have a maximum concentration at approximately three tenths and one sixth of the system length from the injection side, respectively. It is in these places where "clogging" could occur.

8. References

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